Package ‘bbotk’

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**Title**  Black-Box Optimization Toolkit

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**Description**  Provides a common framework for optimization of black-box functions for other packages, e.g. 'mlr3tuning' or 'mlr3fselect'. It offers various optimization methods e.g. grid search, random search, generalized simulated annealing and iterated racing.

**License**  LGPL-3


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**Description**

Provides a common framework for optimization of black-box functions for other packages, e.g. 'mlr3tuning' or 'mlr3fsselect'. It offers various optimization methods e.g. grid search, random search, generalized simulated annealing and iterated racing.

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**See Also**

Useful links:

- [https://bbotk.mlr-org.com](https://bbotk.mlr-org.com)
- [https://github.com/mlr-org/bbotk](https://github.com/mlr-org/bbotk)
Archive

Logging object for objective function evaluations

Description

Container around a `data.table::data.table` which stores all performed function calls of the Objective.

S3 Methods

- `as.data.table(archive)`
  
  ```r
  Archive -> data.table::data.table()
  ```

  Returns a tabular view of all performed function calls of the Objective. The `x_domain` column is unnested to separate columns.

Public fields

- `search_space (paradox::ParamSet)`
  
  Search space of objective.

- `codomain (Codomain)`
  
  Codomain of objective function.

- `start_time (POSIXct)`
  
  Time stamp of when the optimization started. The time is set by the Optimizer.

- `check_values (logical(1))`
  
  Determines if points and results are checked for validity.

- `data (data.table::data.table)`
  
  Contains all performed Objective function calls.

Active bindings

- `n_evals (integer(1))`
  
  Number of evaluations stored in the archive.

- `n_batch (integer(1))`
  
  Number of batches stored in the archive.

- `cols_x (character())`
  
  Column names of search space parameters.

- `cols_y (character())`
  
  Column names of codomain target parameters.

Methods

Public methods:

- `Archive$new()`
- `Archive$add_evals()`
- `Archive$best()`
• Archive$nds_selection()
• Archive$format()
• Archive$print()
• Archive$clear()
• Archive$clone()

Method new(): Creates a new instance of this R6 class.

Usage:
Archive$new(search_space, codomain, check_values = TRUE)

Arguments:
search_space (paradox::ParamSet)
  Specifies the search space for the Optimizer. The paradox::ParamSet describes either a
  subset of the domain of the Objective or it describes a set of parameters together with
  a trafo function that transforms values from the search space to values of the domain.
  Depending on the context, this value defaults to the domain of the objective.
codomain (paradox::ParamSet)
  Specifies codomain of function. Most importantly the tags of each output "Parameter" de-
  fine whether it should be minimized or maximized. The default is to minimize each com-
  ponent.
check_values (logical(1))
  Should x-values that are added to the archive be checked for validity? Search space that is
  logged into archive.

Method add_evals(): Adds function evaluations to the archive table.

Usage:
Archive$add_evals(xdt, xss_trafoed = NULL, ydt)

Arguments:
xdt (data.table::data.table())
  Set of untransformed points / points from the search space. One point per row, e.g. data.table(x1
  = c(1, 3), x2 = c(2, 4)). Column names have to match ids of the search_space. How-
  ever, xdt can contain additional columns.
xss_trafoed (list())
  Transformed point(s) in the domain space.
ydt (data.table::data.table())
  Optimal outcome.

Method best(): Returns the best scoring evaluation(s). For single-crit optimization, the solution
that minimizes / maximizes the objective function. For multi-crit optimization, the Pareto set /
front.

Usage:
Archive$best(batch = NULL, n_select = 1)

Arguments:
batch (integer())
  The batch number(s) to limit the best results to. Default is all batches.
n_select (integer(1L))
   Amount of points to select. Ignored for multi-crit optimization.

Returns: data.table::data.table()

Method nds_selection(): Calculate best points w.r.t. non dominated sorting with hypervolume contribution.

Usage:
Archive$nds_selection(batch = NULL, n_select = 1, ref_point = NULL)

Arguments:
batch (integer())
   The batch number(s) to limit the best points to. Default is all batches.
n_select (integer(1L))
   Amount of points to select.
ref_point (numeric())
   Reference point for hypervolume.

Returns: data.table::data.table()

Method format(): Helper for print outputs.

Usage:
Archive$format()

Method print(): Printer.

Usage:
Archive$print()

Arguments:
... (ignored).

Method clear(): Clear all evaluation results from archive.

Usage:
Archive$clear()

Method clone(): The objects of this class are cloneable with this method.

Usage:
Archive$clone(deep = FALSE)

Arguments:
deep Whether to make a deep clone.
**ArchiveBest**

**Minimal logging object for objective function evaluations**

**Description**

The *ArchiveBest* stores no data but records the best scoring evaluation passed to `$add_evals()`.

The *Archive* API is fully implemented but many parameters are ignored and some methods do nothing. The archive still works with `TerminatorClockTime`, `TerminatorEvals`, `TerminatorNone` and `TerminatorEvals`.

**Super class**

`bbotk::Archive` -> *ArchiveBest*

**Active bindings**

- `n_evals` (integer(1))
  - Number of evaluations stored in the archive.
- `n_batch` (integer(1))
  - Number of batches stored in the archive.

**Methods**

**Public methods:**

- `ArchiveBest$new()`  
- `ArchiveBest$add_evals()`  
- `ArchiveBest$best()`  
- `ArchiveBest$clone()`

**Method** `new()`  

* Creates a new instance of this R6 class.

**Usage:**

`ArchiveBest$new(search_space, codomain, check_values = FALSE)`

**Arguments:**

- `search_space` (*paradox::ParamSet*)  
  - Specifies the search space for the Optimizer. The *paradox::ParamSet* describes either a subset of the domain of the *Objective* or it describes a set of parameters together with a *trafo* function that transforms values from the search space to values of the domain. Depending on the context, this value defaults to the domain of the objective.
- `codomain` (*paradox::ParamSet*)  
  - Specifies codomain of function. Most importantly the tags of each output "Parameter" define whether it should be minimized or maximized. The default is to minimize each component.
- `check_values` (logical(1))  
  - ignored.
Method \texttt{add_evals()}: Stores the best result in \texttt{ydt}.

Usage:
\begin{verbatim}
ArchiveBest$add_evals(xdt, xss_trafoed = NULL, ydt)
\end{verbatim}

Arguments:
\begin{itemize}
\item \texttt{xdt} (\texttt{data.table::data.table()})
  \begin{_description}
  \item Set of untransformed points / points from the \textit{search space}. One point per row, e.g. \texttt{data.table(x1 = c(1, 3), x2 = c(2, 4))}. Column names have to match ids of the \textit{search space}. However, \texttt{xdt} can contain additional columns.
  \end{description}
\item \texttt{xss_trafoed} (\texttt{list()})
  \begin{description}
  \item Transformed point(s) in the \textit{domain space}.
  \end{description}
\item \texttt{ydt} (\texttt{data.table::data.table()})
  \begin{description}
  \item Optimal outcome.
  \end{description}
\end{itemize}

Method \texttt{best()}: Returns the best scoring evaluation. For single-crit optimization, the solution that minimizes / maximizes the objective function. For multi-crit optimization, the Pareto set / front.

Usage:
\begin{verbatim}
ArchiveBest$best(m = NULL)
\end{verbatim}

Arguments:
\begin{itemize}
\item \texttt{m} (\texttt{integer()})
  \begin{description}
  \item ignored.
  \end{description}
\end{itemize}

Returns: \texttt{data.table::data.table()}

Method \texttt{clone()}: The objects of this class are cloneable with this method.

Usage:
\begin{verbatim}
ArchiveBest$clone(deep = FALSE)
\end{verbatim}

Arguments:
\begin{itemize}
\item \texttt{deep} Whether to make a deep clone.
\end{itemize}

\begin{longtable}{ll}
\hline
\texttt{bb_optimize} & \textit{Black-Box Optimization} \\
\hline
\end{longtable}

\textbf{Description}

This function optimizes a function or \texttt{Objective} with a given method.

\textbf{Usage}

\begin{verbatim}
bb_optimize(
  x,
  method = "random_search",
  max_evals = 1000,
  max_time = NULL,
\end{verbatim}
bb_optimize

```r

## S3 method for class 'function'
bb_optimize(
  x,
  method = "random_search",
  max_evals = 1000,
  max_time = NULL,
  lower = NULL,
  upper = NULL,
  maximize = FALSE,
  ...
)

## S3 method for class 'Objective'
bb_optimize(
  x,
  method = "random_search",
  max_evals = 1000,
  max_time = NULL,
  search_space = NULL,
  ...
)

Arguments

- **x** (function | Objective).
- **method** (character(1) | Optimizer)
  Key to retrieve optimizer from mlr_optimizers dictionary or Optimizer.
- **max_evals** (integer(1))
  Number of allowed evaluations.
- **max_time** (integer(1))
  Maximum allowed time in seconds.
- **...** (named list())
  Named arguments passed to objective function. Ignored if Objective is optimized.
- **lower** (numeric())
  Lower bounds on the parameters. If named, names are used to create the domain.
- **upper** (numeric())
  Upper bounds on the parameters.
- **maximize** (logical())
  Logical vector used to create the codomain e.g. c(TRUE, FALSE) -> ps(y1 = p_dbl(tags = "maximize"), y2 = pd_dbl(tags = "minimize")). If named, names are used to create the codomain.
- **search_space** (paradox::ParamSet).
```
Value

list of

• "par" - Best found parameters
• "value" - Optimal outcome
• "instance" - OptimInstanceSingleCrit | OptimInstanceMultiCrit

Note

If both max_evals and max_time are NULL, TerminatorNone is used. This is useful if the Optimizer can terminate itself. If both are given, TerminatorCombo is created and the optimization stops if the time or evaluation budget is exhausted.

Examples

```r
# function and bounds
fun = function(xs) {
  -(xs[[1]] - 2)^2 - (xs[[2]] + 3)^2 + 10
}

bb_optimize(fun, lower = c(-10, -5), upper = c(10, 5), max_evals = 10)

# function and constant
fun = function(xs, c) {
  -(xs[[1]] - 2)^2 - (xs[[2]] + 3)^2 + c
}

bb_optimize(fun, lower = c(-10, -5), upper = c(10, 5), max_evals = 10, c = 1)

# objective
fun = function(xs) {
  c(z = -(xs[[1]] - 2)^2 - (xs[[2]] + 3)^2 + 10)
}

# define domain and codomain using a `ParamSet` from paradox
domain = ps(x1 = p_dbl(-10, 10), x2 = p_dbl(-5, 5))
codomain = ps(z = p_dbl(tags = "minimize"))
optimizer = ObjectiveRFun$new(fun, domain, codomain)

bb_optimize(objective, method = "random_search", max_evals = 10)
```

---

branin  

Branin Function

Description

Augmented 2-D Branin function with fidelity parameter.
Codomain

Usage
branin(xs)

Arguments
xs List with the input for a single point (e.g. list(x1 = 1, x2 = 2, fidelity = 0.5)).

Value
list(1)

Source

Examples
branin(list(x1 = 12, x2 = 2, fidelity = 1))

Codomain  Codomain of Function

Description
A set of Param objects defining the codomain of a function. The parameter set must contain at least one target parameter tagged with "minimize" or "maximize". The codomain may contain extra parameters which are ignored when calling the Archive methods $best(), $nds_selection() and $cols_y. This class is usually constructed internally from a paradox::ParamSet when Objective is initialized.

Super class
paradox::ParamSet -> Codomain

Active bindings
is_target (named logical())
   Position is TRUE for target Params.
target_length (integer())
   Returns number of target Params.
target_ids (character())
   Number of contained target Params.
target_tags (named list() of character())
   Tags of target Params.
maximization_to_minimization (integer())
   Returns a numeric vector with values -1 and 1. Multiply with the outcome of a maximization problem to turn it into a minimization problem.
Methods

Public methods:

- `Codomain$new()`
- `Codomain$clone()`

**Method new():** Creates a new instance of this R6 class.

**Usage:**
`Codomain$new(params = named_list())`

**Arguments:**
- `params` (list())
  List of `Param`, named with their respective ID. Parameters are cloned.

**Method clone():** The objects of this class are cloneable with this method.

**Usage:**
`Codomain$clone(deep = FALSE)`

**Arguments:**
- `deep` Whether to make a deep clone.

Examples

```r
# define objective function
fun = function(xs) {
  c(y = -(xs[[1]] - 2)^2 - (xs[[2]] + 3)^2 + 10)
}

# set domain
domain = ps(
  x1 = p_dbl(-10, 10),
  x2 = p_dbl(-5, 5)
)

# set codomain
codomain = ps(
  y = p_dbl(tags = "maximize"),
  time = p_dbl()
)

# create Objective object
objective = ObjectiveRFun$new(
  fun = fun,
  domain = domain,
  codomain = codomain,
  properties = "deterministic"
)
```
is_dominated  

### Calculate which points are dominated

**Description**

Returns which points from a set are dominated by another point in the set.

**Usage**

```r
is_dominated(ymat)
```

**Arguments**

- `ymat` (matrix()): A numeric matrix. Each column (!) contains one point.

**mlr_optimizers  

Dictionary of Optimizer

**Description**

A simple `mlr3misc::Dictionary` storing objects of class `Optimizer`. Each optimizer has an associated help page, see `mlr_optimizer_[id]`.

This dictionary can get populated with additional optimizer by add-on packages.

For a more convenient way to retrieve and construct optimizer, see `opt()`/`opts()`.

**Format**

R6::R6Class object inheriting from `mlr3misc::Dictionary`.

**Methods**

See `mlr3misc::Dictionary`.

**S3 methods**

- as.data.table(dict, ..., objects = FALSE)

  ```r
  mlr3misc::Dictionary -> data.table::data.table()
  ```

  Returns a `data.table::data.table()` with fields "key", "label", "param_classes", "properties" and "packages" as columns. If `objects` is set to TRUE, the constructed objects are returned in the list column named `object`.

**See Also**

Sugar functions: `opt()`, `opts()`
Examples

```r
as.data.table(mlr_optimizers)
mlr_optimizers$get("random_search")
opt("random_search")
```

---

### Optimization via Covariance Matrix Adaptation Evolution Strategy

#### Description

OptimizerCmaes class that implements CMA-ES. Calls `adagio::pureCMAES()` from package `adagio`. The algorithm is typically applied to search space dimensions between three and fifty. Lower search space dimensions might crash.

#### Dictionary

This Optimizer can be instantiated via the dictionary `mlr_optimizers` or with the associated sugar function `opt()`:

```r
mlr_optimizers$get("cmaes")
opt("cmaes")
```

#### Parameters

- **sigma** numeric(1)
- **start_values** character(1)
  
  Create random start values or based on center of search space? In the latter case, it is the center of the parameters before a trafo is applied.

For the meaning of the control parameters, see `adagio::pureCMAES()`. Note that we have removed all control parameters which refer to the termination of the algorithm and where our terminators allow to obtain the same behavior.

#### Progress Bars

 `$optimize()` supports progress bars via the package `progressr` combined with a Terminator. Simply wrap the function in `progressr::with_progress()` to enable them. We recommend to use package `progress` as backend; enable with `progressr::handlers("progress")`.

#### Super class

`bbotk::Optimizer` -> `OptimizerCmaes`
Methods

**Public methods:**

- `OptimizerCmaes$new()`
- `OptimizerCmaes$clone()`

**Method `new()`**: Creates a new instance of this R6 class.

**Usage:**
```
OptimizerCmaes$new()
```

**Method `clone()`**: The objects of this class are cloneable with this method.

**Usage:**
```
OptimizerCmaes$clone(deep = FALSE)
```

**Arguments:**
- `deep` Whether to make a deep clone.

**Examples**

```r
if (requireNamespace("adagio")) {
  search_space = domain = ps(
    x1 = p_dbl(-10, 10),
    x2 = p_dbl(-5, 5)
  )
  codomain = ps(y = p_dbl(tags = "maximize"))

  objective_function = function(xs) {
    c(y = -(xs[[1]] - 2)^2 - (xs[[2]] + 3)^2 + 10)
  }

  objective = ObjectiveRFun$new(
    fun = objective_function,
    domain = domain,
    codomain = codomain)

  instance = OptimInstanceSingleCrit$new(
    objective = objective,
    search_space = search_space,
    terminator = trm("evals", n_evals = 10))

  optimizer = opt("cmaes")

  # modifies the instance by reference
  optimizer$optimize(instance)

  # returns best scoring evaluation
  instance$result

  # allows access of data.table of full path of all evaluations
  as.data.table(instance$archive$data)
}
```
OptimizerDesignPoints class that implements optimization w.r.t. fixed design points. We simply search over a set of points fully specified by the user. The points in the design are evaluated in order as given.

In order to support general termination criteria and parallelization, we evaluate points in a batch-fashion of size batch_size. Larger batches mean we can parallelize more, smaller batches imply a more fine-grained checking of termination criteria.

This Optimizer can be instantiated via the dictionary mlr_optimizers or with the associated sugar function opt():

```r
mlr_optimizers$get("design_points")
opt("design_points")
```

Parameters

- **batch_size** integer(1)
  - Maximum number of configurations to try in a batch.
- **design** data.table::data.table
  - Design points to try in search, one per row.

Progress Bars

$optimize() supports progress bars via the package progressr combined with a Terminator. Simply wrap the function in progressr::with_progress() to enable them. We recommend to use package progress as backend; enable with progressr::handlers("progress").

Super class

bbotk::Optimizer -> OptimizerDesignPoints

Methods

- Public methods:
  - OptimizerDesignPoints$new()
  - OptimizerDesignPoints$clone()

Method new(): Creates a new instance of this R6 class.

Usage:
OptimizerDesignPoints$new()

**Method** `clone()`: The objects of this class are cloneable with this method.

**Usage:**
OptimizerDesignPoints$clone(deep = FALSE)

**Arguments:**
- `deep` Whether to make a deep clone.

**Examples**

```r
library(data.table)
search_space = domain = ps(x = p_dbl(lower = -1, upper = 1))
codomain = ps(y = p_dbl(tags = "minimize"))

objective_function = function(xs) {
  list(y = as.numeric(xs)^2)
}

objective = ObjectiveRFun$new(
  fun = objective_function,
  domain = domain,
  codomain = codomain)

instance = OptimInstanceSingleCrit$new(
  objective = objective,
  search_space = search_space,
  terminator = trm("evals", n_evals = 10))

design = data.table(x = c(0, 1))

optimizer = opt("design_points", design = design)

# Modifies the instance by reference
optimizer$optimize(instance)

# Returns best scoring evaluation
instance$result

# Allows access of data.table of full path of all evaluations
as.data.table(instance$archive)
```

---

**mlr_optimizers_gensa  Optimization via Generalized Simulated Annealing**

**Description**

OptimizerGenSA class that implements generalized simulated annealing. Calls `GenSA::GenSA()` from package `GenSA`. 
Dictionary

This Optimizer can be instantiated via the dictionary mlr_optimizers or with the associated sugar function opt():

```r
mlr_optimizers$get("genSA")
opt("genSA")
```

Parameters

- smooth logical(1)
- temperature numeric(1)
- acceptance.param numeric(1)
- verbose logical(1)
- trace.mat logical(1)

For the meaning of the control parameters, see `GenSA::GenSA()`. Note that we have removed all control parameters which refer to the termination of the algorithm and where our terminators allow to obtain the same behavior.

Progress Bars

`$optimize()` supports progress bars via the package `progressr` combined with a Terminator. Simply wrap the function in `progressr::with_progress()` to enable them. We recommend to use package `progress` as backend; enable with `progressr::handlers("progress")`.

Super class

`bbotk::Optimizer` -> OptimizerGenSA

Methods

Public methods:

- `OptimizerGenSA$new()`
- `OptimizerGenSA$clone()`

Method `new()`: Creates a new instance of this R6 class.

Usage:

```r
OptimizerGenSA$new()
```

Method `clone()`: The objects of this class are cloneable with this method.

Usage:

```r
OptimizerGenSA$clone(deep = FALSE)
```

Arguments:

deep    Whether to make a deep clone.
Source


Examples

```r
if (requireNamespace("GenSA")) {

  search_space = domain = ps(x = p_dbl(lower = -1, upper = 1))
  codomain = ps(y = p_dbl(tags = 'minimize'))

  objective_function = function(xs) {
    list(y = as.numeric(xs)^2)
  }

  objective = ObjectiveRFun$new(
    fun = objective_function,
    domain = domain,
    codomain = codomain)

  instance = OptimInstanceSingleCrit$new(
    objective = objective,
    search_space = search_space,
    terminator = trm("evals", n_evals = 10))

  optimizer = opt("cmaes")

  # Modifies the instance by reference
  optimizer$optimize(instance)

  # Returns best scoring evaluation
  instance$result

  # Allows access of data.table of full path of all evaluations
  as.data.table(instance$archive$data)
}
```

Optimization via Grid Search

OptimizerGridSearch class that implements grid search. The grid is constructed as a Cartesian product over discretized values per parameter, see `paradox::generate_design_grid()`. The points of the grid are evaluated in a random order.
In order to support general termination criteria and parallelization, we evaluate points in a batch-fasion of size \texttt{batch\_size}. Larger batches mean we can parallelize more, smaller batches imply a more fine-grained checking of termination criteria.

**Dictionary**

This Optimizer can be instantiated via the dictionary \texttt{mlr\_optimizers} or with the associated sugar function \texttt{opt()}:

\begin{verbatim}
mlr_optimizers$get("grid_search")
\end{verbatim}

\begin{verbatim}
opt("grid_search")
\end{verbatim}

### Parameters

- \texttt{resolution integer(1)}
  - Resolution of the grid, see \texttt{paradox::generate\_design\_grid()}.

- \texttt{param\_resolutions named integer()}
  - Resolution per parameter, named by parameter ID, see \texttt{paradox::generate\_design\_grid()}.

- \texttt{batch\_size integer(1)}
  - Maximum number of points to try in a batch.

### Progress Bars

\$optimize() supports progress bars via the package \texttt{progressr} combined with a Terminator. Simply wrap the function in \texttt{progressr::with\_progress()} to enable them. We recommend to use package \texttt{progress} as backend; enable with \texttt{progressr::handlers("progress")}.

### Super class

\texttt{bbotk::Optimizer -> OptimizerGridSearch}

### Methods

**Public methods:**

- \texttt{OptimizerGridSearch$new()}
- \texttt{OptimizerGridSearch$clone()}  

**Method \texttt{new()}:** Creates a new instance of this \texttt{R6} class.

\begin{verbatim}
OptimizerGridSearch$new()
\end{verbatim}

**Method \texttt{clone()}:** The objects of this class are cloneable with this method.

\begin{verbatim}
OptimizerGridSearch$clone()
\end{verbatim}

\texttt{Arguments:}

- \texttt{deep} Whether to make a deep clone.
Examples

```r
search_space = domain = ps(x = p_dbl(lower = -1, upper = 1))

codomain = ps(y = p_dbl(tags = "minimize"))

objective_function = function(xs) {
  list(y = as.numeric(xs)^2)
}

objective = ObjectiveRFun$new(
  fun = objective_function,
  domain = domain,
  codomain = codomain)

instance = OptimInstanceSingleCrit$new(
  objective = objective,
  search_space = search_space,
  terminator = trm("evals", n_evals = 10))

optimizer = opt("grid_search")
# modifies the instance by reference
optimizer$optimize(instance)
# returns best scoring evaluation
instance$result
# allows access of data.table of full path of all evaluations
as.data.table(instance$archive$data)
```

---

**mlr_optimizers_irace**  
*Optimization via Iterated Racing*

**Description**

OptimizerIrace class that implements iterated racing. Calls `irace::irace()` from package `irace`.

**Parameters**

- **instances list()**
  A list of instances where the configurations executed on.

- **targetRunnerParallel function()**
  A function that executes the objective function with a specific parameter configuration and instance. A default function is provided, see section "Target Runner and Instances".

For the meaning of all other parameters, see `irace::defaultScenario()`. Note that we have removed all control parameters which refer to the termination of the algorithm. Use `TerminatorEvals` instead. Other terminators do not work with `OptimizerIrace`.
Target Runner and Instances

The irace package uses a targetRunner script or R function to evaluate a configuration on a particular instance. Usually it is not necessary to specify a targetRunner function when using OptimizerIrace. A default function is used that forwards several configurations and instances to the user defined objective function. As usually, the user defined function has a xs, xss or xdt parameter depending on the used Objective class. For irace, the function needs an additional instances parameter.

fun = function(xs, instances) {
  # function to evaluate configuration in `xs` on instance `instances`
}

Archive

The Archive holds the following additional columns:

- "race" (integer(1))  
  Race iteration.
- "step" (integer(1))  
  Step number of race.
- "instance" (integer(1))  
  Identifies instances across races and steps.
- "configuration" (integer(1))  
  Identifies configurations across races and steps.

Result

The optimization result (instance$result) is the best performing elite of the final race. The reported performance is the average performance estimated on all used instances.

Dictionary

This Optimizer can be instantiated via the dictionary mlr_optimizers or with the associated sugar function opt():

mlr_optimizers$get("irace")
opt("irace")

Progress Bars

$optimize() supports progress bars via the package progressr combined with a Terminator. Simply wrap the function in progressr::with_progress() to enable them. We recommend to use package progress as backend; enable with progressr::handlers("progress").

Super class

bbotk::Optimizer -> OptimizerIrace
Methods

Public methods:
• OptimizerIrace$new()
• OptimizerIrace$clone()

Method new(): Creates a new instance of this R6 class.

Usage:
OptimizerIrace$new()

Method clone(): The objects of this class are cloneable with this method.

Usage:
OptimizerIrace$clone(deep = FALSE)

Arguments:
depth Whether to make a deep clone.

Source

Examples
library(data.table)

search_space = domain = ps(
  x1 = p_dbl(-5, 10),
  x2 = p_dbl(0, 15)
)

codomain = ps(y = p_dbl(tags = "minimize"))

# branin function with noise
# the noise generates different instances of the branin function
# the noise values are passed via the 'instances' parameter
fun = function(xdt, instances) {
  a = 1
  b = 5.1 / (4 * (pi^2))
  c = 5 / pi
  r = 6
  s = 10
  t = 1 / (8 * pi)

data.table(y = {
  a * ((xdt["x2"] -
    b * (xdt["x1"]^2)) +
  c * xdt["x1"] - r)^2) +
  ((s * (1 - t)) * cos(xdt["x1"])) +
  unlist(instances)))
mlr_optimizers_nloptr

### Optimization via Non-linear Optimization

**Description**

OptimizerNloptr class that implements non-linear optimization. Calls `nloptr::nloptr()` from package `nloptr`.

**Parameters**

- `algorithm` character(1)
- `eval_g_ineq` function()
- `xtol_rel` numeric(1)
- `xtol_abs` numeric(1)
- `ftol_rel` numeric(1)
- `ftol_abs` numeric(1)
- `start_values` character(1)

Create random start values or based on center of search space? In the latter case, it is the center of the parameters before a trafo is applied.

For the meaning of the control parameters, see `nloptr::nloptr()` and `nloptr::nloptr.print.options()`. The termination conditions `stopval`, `maxtime` and `maxeval` of `nloptr::nloptr()` are deactivated and replaced by the Terminator subclasses. The x and function value tolerance termination conditions (`xtol_rel = 10^{-4}`, `xtol_abs = rep(0.0, length(x0))`, `ftol_rel = 0.0` and `ftol_abs = 0.0`) are still available and implemented with their package defaults. To deactivate these conditions, set them to `-1`.
Progress Bars
$optimize$ supports progress bars via the package \texttt{progressr} combined with a \texttt{Terminator}. Simply wrap the function in \texttt{progressr::with_progress()} to enable them. We recommend to use package \texttt{progress} as backend; enable with \texttt{progressr::handlers("progress")}.

Super class

\texttt{bbotk::Optimizer} \rightarrow \texttt{OptimizerNLoptr}

Methods

Public methods:
- \texttt{OptimizerNLoptr$\text{new}()} \\
- \texttt{OptimizerNLoptr$\text{clone}()}

Method \texttt{new}(): Creates a new instance of this R6 class.

Usage:
\texttt{OptimizerNLoptr$\text{new}()}

Method \texttt{clone}(): The objects of this class are cloneable with this method.

Usage:
\texttt{OptimizerNLoptr$\text{clone}() (deep = FALSE)}

Arguments:
- \texttt{deep} Whether to make a deep clone.

Source


Examples

```r
if (requireNamespace("nloptr")) {
  search_space = domain = ps(x = p_dbl(lower = -1, upper = 1))
  codomain = ps(y = p_dbl(tags = "minimize"))
  objective_function = function(xs) {
    list(y = as.numeric(xs)^2)
  }
  objective = ObjectiveRFun$new(
    fun = objective_function,
    domain = domain,
    codomain = codomain)
}
```
# We use the internal termination criterion xtol_rel
terminator = trm("none")
instance = OptimInstanceSingleCrit$new(
  objective = objective,
  search_space = search_space,
  terminator = terminator)

optimizer = opt("nloptr", algorithm = "NLOPT_LN_BOBYQA")

# Modifies the instance by reference
optimizer$optimize(instance)

# Returns best scoring evaluation
instance$result

# Allows access of data.table of full path of all evaluations
as.data.table(instance$archive)

mlr_optimizers_random_search

Optimization via Random Search

Description

OptimizerRandomSearch class that implements a simple Random Search.
In order to support general termination criteria and parallelization, we evaluate points in a batch-
fashion of size batch_size. Larger batches mean we can parallelize more, smaller batches imply a
more fine-grained checking of termination criteria.

Dictionary

This Optimizer can be instantiated via the dictionary mlr_optimizers or with the associated sugar
function opt():

mlr_optimizers$get("random_search")
opt("random_search")

Parameters

batch_size integer(1)
  Maximum number of points to try in a batch.

Progress Bars

$optimize() supports progress bars via the package progressr combined with a Terminator. Sim-
ply wrap the function in progressr::with_progress() to enable them. We recommend to use
package progress as backend; enable with progressr::handlers("progress").
Super class

\texttt{bbotk::Optimizer} \rightarrow \texttt{OptimizerRandomSearch}

Methods

Public methods:

- \texttt{OptimizerRandomSearch$new()}
- \texttt{OptimizerRandomSearch$clone()}

Method \texttt{new()}: Creates a new instance of this R6 class.

Usage:

\texttt{OptimizerRandomSearch$new()}

Method \texttt{clone()}: The objects of this class are cloneable with this method.

Usage:

\texttt{OptimizerRandomSearch$clone(deep = FALSE)}

Arguments:

depth Whether to make a deep clone.

Source


Examples

\begin{verbatim}
search_space = domain = ps(x = p_dbl(lower = -1, upper = 1))

codomain = ps(y = p_dbl(tags = "minimize"))

objective_function = function(xs) {
  list(y = as.numeric(xs)^2)
}

objective = ObjectiveRFun$new(
  fun = objective_function,
  domain = domain,
  codomain = codomain)

instance = OptimInstanceSingleCrit$new(
  objective = objective,
  search_space = search_space,
  terminator = trm("evals", n_evals = 10))

optimizer = opt("random_search")

# modifies the instance by reference
\end{verbatim}
mlr_terminators

optimizer$optimize(instance)

# returns best scoring evaluation
instance$result

# allows access of data.table of full path of all evaluations
as.data.table(instance$archive$data)

description

A simple mlr3misc::Dictionary storing objects of class Terminator. Each terminator has an associated help page, see mlr_terminators_[id].

This dictionary can get populated with additional terminators by add-on packages.

For a more convenient way to retrieve and construct terminator, see trm()/trms().

format

R6::R6Class object inheriting from mlr3misc::Dictionary.

methods

See mlr3misc::Dictionary.

S3 methods

• as.data.table(dict, ..., objects = FALSE)
  mlr3misc::Dictionary -> data.table::data.table()
  Returns a data.table::data.table() with fields "key", "label", "properties" and "unit" as columns. If objects is set to TRUE, the constructed objects are returned in the list column named object.

see also

Sugar functions: trm(), trms()


examples

as.data.table(mlr_terminators)
mlr_terminators$get("evals")
trm("evals", n_evals = 10)
**Description**

Class to terminate the optimization after a fixed time point has been reached (as reported by `Sys.time()`).

**Dictionary**

This Terminator can be instantiated via the dictionary `mlr_terminators` or with the associated sugar function `trm()`:

```r
mlr_terminators$get("clock_time")
trm("clock_time")
```

**Parameters**

- `stop_time` `POSIXct(1)`
  Terminator stops after this point in time.

**Super class**

`bbotk::Terminator` -> `TerminatorClockTime`

**Methods**

**Public methods:**

- `TerminatorClockTime$new()`
- `TerminatorClockTime$is_terminated()`
- `TerminatorClockTime$clone()`

**Method** `new()`: Creates a new instance of this R6 class.

*Usage:*

`TerminatorClockTime$new()`

**Method** `is_terminated()`: Is TRUE iff the termination criterion is positive, and FALSE otherwise.

*Usage:*

`TerminatorClockTime$is_terminated(archive)`

*Arguments:*

- `archive` (Archive).

*Returns:*

- logical(1).

**Method** `clone()`: The objects of this class are cloneable with this method.
**Usage:**
TerminatorClockTime$clone(deep = FALSE)

**Arguments:**
deep  Whether to make a deep clone.

**See Also**

**Examples**
```r
stop_time = as.POSIXct("2030-01-01 00:00:00")
trm("clock_time", stop_time = stop_time)
```

---

**mlr_terminators_combo  Combine Terminators**

**Description**
This class takes multiple Terminators and terminates as soon as one or all of the included terminators are positive.

**Dictionary**
This Terminator can be instantiated via the dictionary mlr_terminators or with the associated sugar function `trm()`:

```r
mlr_terminators$get("combo")
trm("combo")
```

**Parameters**
- any logical(1)
  Terminate iff any included terminator is positive? (not all). Default is TRUE.

**Super class**
bbotk::Terminator -> TerminatorCombo

**Public fields**
- terminators (list())
  List of objects of class Terminator.
Methods

Public methods:

- `TerminatorCombo$new()`
- `TerminatorCombo$is_terminated()`
- `TerminatorCombo$print()`
- `TerminatorCombo$remaining_time()`
- `TerminatorCombo$status_long()`
- `TerminatorCombo$clone()`

Method `new()`: Creates a new instance of this R6 class.

Usage:
`TerminatorCombo$new(terminators = list(TerminatorNone$new()))`

Arguments:
- `terminators` (list())
  List of objects of class `Terminator`.

Method `is_terminated()`: Is TRUE iff the termination criterion is positive, and FALSE otherwise.

Usage:
`TerminatorCombo$is_terminated(archive)`

Arguments:
- `archive` (Archive).

Returns: logical(1).

Method `print()`: Printer.

Usage:
`TerminatorCombo$print(...)`

Arguments:
- `...` (ignored).

Method `remaining_time()`: Returns the remaining runtime in seconds. If `any = TRUE`, the remaining runtime is determined by the time-based terminator with the shortest time remaining. If non-time-based terminators are used and `any = FALSE`, the the remaining runtime is always Inf.

Usage:
`TerminatorCombo$remaining_time(archive)`

Arguments:
- `archive` (Archive).

Returns: integer(1).

Method `status_long()`: Returns `max_steps` and `current_steps` for each terminator.

Usage:
`TerminatorCombo$status_long(archive)`
mlr_terminators_evals

Arguments:
archive (Archive).

Returns: data.table::data.table.

Method clone(): The objects of this class are cloneable with this method.

Usage:
TerminatorCombo$clone(deep = FALSE)

Arguments:
deep Whether to make a deep clone.

See Also

Examples

trm("combo",
    list(trm("clock_time", stop_time = Sys.time() + 60),
         trm("evals", n_evals = 10)), any = FALSE
)

mlr_terminators_evals  Terminator that stops after a number of evaluations

Description

Class to terminate the optimization depending on the number of evaluations. An evaluation is defined by one resampling of a parameter value. The total number of evaluations $B$ is defined as

$$B = n_{evals} + k \times D$$

where $D$ is the dimension of the search space.

Dictionary

This Terminator can be instantiated via the dictionary mlr_terminators or with the associated sugar function trm():

mlr_terminators$get("evals")
trm("evals")
Parameters

\begin{itemize}
  \item n_evals \text{integer}(1)
    \begin{itemize}
      \item See formula above. Default is 100.
    \end{itemize}
  \item k \text{integer}(1)
    \begin{itemize}
      \item See formula above. Default is 0.
    \end{itemize}
\end{itemize}

Super class

\texttt{bbotk::Terminator} -> \texttt{TerminatorEvals}

Methods

Public methods:

\begin{itemize}
  \item \texttt{TerminatorEvals$new()}
  \item \texttt{TerminatorEvals$\text{is\_terminated}()}
  \item \texttt{TerminatorEvals$\text{clone}()}
\end{itemize}

Method \texttt{new()}: Creates a new instance of this \texttt{R6} class.

Usage:
\texttt{TerminatorEvals$new()}

Method \texttt{is\_terminated()}: Is \texttt{TRUE} iff the termination criterion is positive, and \texttt{FALSE} otherwise.

Usage:
\texttt{TerminatorEvals$\text{is\_terminated}(archive)}

Arguments:
archive (\texttt{Archive}).

Returns: \texttt{logical(1)}.

Method \texttt{clone()}: The objects of this class are cloneable with this method.

Usage:
\texttt{TerminatorEvals$\text{clone}(\text{deep} = \text{FALSE})}

Arguments:
\texttt{deep} Whether to make a deep clone.

See Also

Other Terminator: \texttt{Terminator, mlr\_terminators\_clock\_time, mlr\_terminators\_combo, mlr\_terminators\_none, mlr\_terminators\_perf\_reached, mlr\_terminators\_run\_time, mlr\_terminators\_stagnation\_batch, mlr\_terminators\_stagnation, mlr\_terminators}
Examples

TerminatorEvals$new()

# 5 evaluations in total
trm("evals", n_evals = 5)

# 3 * [dimension of search space] evaluations in total
trm("evals", n_evals = 0, k = 3)

# (3 * [dimension of search space] + 1) evaluations in total
trm("evals", n_evals = 1, k = 3)

---

mlr_terminators_none  None Terminator

Description

Mainly useful for optimization algorithms where the stopping is inherently controlled by the algorithm itself (e.g. OptimizerGridSearch).

Dictionary

This Terminator can be instantiated via the dictionary mlr_terminators or with the associated sugar function trm():

mlr_terminators$get("none")
trm("none")

Super class

bbotk::Terminator -> TerminatorNone

Methods

Public methods:
- TerminatorNone$new()
- TerminatorNone$is_terminated()
- TerminatorNone$clone()

Method new(): Creates a new instance of this R6 class.
Usage:
TerminatorNone$new()

Method is_terminated(): Is TRUE iff the termination criterion is positive, and FALSE otherwise.
Usage:
TerminatorNone$is_terminated(archive)
Arguments:
archive (Archive).

Returns: logical(1).

Method clone(): The objects of this class are cloneable with this method.

Usage:
TerminatorNone$clone(deep = FALSE)

Arguments:
deep Whether to make a deep clone.

See Also

mlr_terminators_perf_reached

Performance Level Terminator

Description
Class to terminate the optimization after a performance level has been hit.

Dictionary
This Terminator can be instantiated via the dictionary mlr_terminators or with the associated sugar function trm():

mlr_terminators$get("perf_reached")
trm("perf_reached")

Parameters
level numeric(1)
Performance level that needs to be reached. Default is 0. Terminates if the performance exceeds (respective measure has to be maximized) or falls below (respective measure has to be minimized) this value.

Super class
bbotk::Terminator -> TerminatorPerfReached
Methods

Public methods:

- TerminatorPerfReached$new()
- TerminatorPerfReached$is_terminated()
- TerminatorPerfReached$clone()

Method new(): Creates a new instance of this R6 class.

Usage:
TerminatorPerfReached$new()

Method is_terminated(): Is TRUE iff the termination criterion is positive, and FALSE otherwise.

Usage:
TerminatorPerfReached$is_terminated(archive)

Arguments:
archive (Archive).

Returns: logical(1).

Method clone(): The objects of this class are cloneable with this method.

Usage:
TerminatorPerfReached$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

See Also

Other Terminator: Terminator, mlr_terminators_clock_time, mlr_terminators_combo, mlr_terminators_evals,
mlr_terminators_none, mlr_terminators_run_time, mlr_terminators_stagnation_batch,
mlr_terminators_stagnation, mlr_terminators

Examples

TerminatorPerfReached$new()
trm("perf_reached")
Run Time Terminator

Description
Class to terminate the optimization after the optimization process took a number of seconds on the clock.

Dictionary
This Terminator can be instantiated via the dictionary mlr_terminators or with the associated sugar function trm():

```
mlr_terminators$get("run_time")
trm("run_time")
```

Parameters
secs numeric(1)
Maximum allowed time, in seconds, default is 100.

Super class
```
bbotk::Terminator -> TerminatorRunTime
```

Methods

Public methods:
- TerminatorRunTime$new()
- TerminatorRunTime$is_terminated()
- TerminatorRunTime$clone()

Method `new()`: Creates a new instance of this R6 class.
Usage:
```
TerminatorRunTime$new()
```

Method `is_terminated()`: Is TRUE iff the termination criterion is positive, and FALSE otherwise.
Usage:
```
TerminatorRunTime$is_terminated(archive)
```
Arguments:
archive (Archive).
Returns: logical(1).

Method `clone()`: The objects of this class are cloneable with this method.
**Usage:**
TerminatorRunTime$clone(deep = FALSE)

**Arguments:**
deep Whether to make a deep clone.

**Note**
This terminator only works if archive$start_time is set. This is usually done by the Optimizer.

**See Also**

**Examples**
trm("run_time", secs = 1800)

---

---

**Description**
Class to terminate the optimization after the performance stagnates, i.e. does not improve more than threshold over the last iters iterations.

**Dictionary**
This Terminator can be instantiated via the dictionary mlr_terminators or with the associated sugar function trm():

```
mlr_terminators$get("stagnation")
trm("stagnation")
```

**Parameters**

- `iters integer(1)`
  Number of iterations to evaluate the performance improvement on, default is 10.
- `threshold numeric(1)`
  If the improvement is less than threshold, optimization is stopped, default is 0.

**Super class**
`bbotk::Terminator` -> TerminatorStagnation
Methods

Public methods:

• TerminatorStagnation$new()
• TerminatorStagnation$is_terminated()
• TerminatorStagnation(clone)

Method new(): Creates a new instance of this R6 class.

Usage:
TerminatorStagnation$new()

Method is_terminated(): Is TRUE iff the termination criterion is positive, and FALSE otherwise.

Usage:
TerminatorStagnation$is_terminated(archive)

Arguments:
archive (Archive).

Returns: logical(1).

Method clone(): The objects of this class are cloneable with this method.

Usage:
TerminatorStagnation$clone(deep = FALSE)

Arguments:
deep Whether to make a deep clone.

See Also

Other Terminator: Terminator, mlr_terminators_clock_time, mlr_terminators_combo, mlr_terminators_evals,
mlr_terminators_none, mlr_terminators_perf_reached, mlr_terminators_run_time, mlr_terminators_stagnation_batch,
mlr_terminators

Examples

TerminatorStagnation$new()
trm("stagnation", iters = 5, threshold = 1e-5)
mlr_terminators_stagnation_batch

Terminator that stops when optimization does not improve

Description

Class to terminate the optimization after the performance stagnates, i.e. does not improve more than threshold over the last $n$ batches.

Dictionary

This Terminator can be instantiated via the dictionary mlr_terminators or with the associated sugar function trm():

```
mlr_terminators$get("stagnation_batch")
trm("stagnation_batch")
```

Parameters

- $n$ integer(1)
  Number of batches to evaluate the performance improvement on, default is 1.
- threshold numeric(1)
  If the improvement is less than threshold, optimization is stopped, default is 0.

Super class

bbotk::Terminator -> TerminatorStagnationBatch

Methods

Public methods:

- TerminatorStagnationBatch$new()
- TerminatorStagnationBatch$clone()

Method new(): Creates a new instance of this R6 class.

Usage:
```
TerminatorStagnationBatch$new()
```

Method is_terminated(): Is TRUE iff the termination criterion is positive, and FALSE otherwise.

Usage:
```
TerminatorStagnationBatch$is_terminated(archive)
```

Arguments:
archive (Archive).
Returns: logical(1).

Method clone(): The objects of this class are cloneable with this method.

Usage:
TerminatorStagnationBatch$clone(deep = FALSE)

Arguments:
deep  Whether to make a deep clone.

See Also


Examples

TerminatorStagnationBatch$new()
trm("stagnation_batch", n = 1, threshold = 1e-5)

---

**Objective**  
(*Objective function with domain and co-domain*)

**Description**

Describes a black-box objective function that maps an arbitrary domain to a numerical codomain.

**Technical details**

Objective objects can have the following properties: "noisy", "deterministic", "single-crit" and "multi-crit".

**Public fields**

- id (character(1)).
- properties (character(1)).
- domain (paradox::ParamSet)
  - Specifies domain of function, hence its input parameters, their types and ranges.
- codomain (paradox::ParamSet)
  - Specifies codomain of function, hence its feasible values.
- constants (paradox::ParamSet)
  - Changeable constants or parameters that are not subject to tuning can be stored and accessed here. Set constant values are passed to $.eval() and $.eval_many() as named arguments.
- check_values (logical(1))
Active bindings

xdim (integer(1))
   Dimension of domain.

ydim (integer(1))
   Dimension of codomain.

Methods

**Public methods:**

- `Objective$new()`
- `Objective/format()`
- `Objective/print()`
- `Objective/eval()`
- `Objective/eval_many()`
- `Objective/eval_dt()`
- `Objective/clone()`

**Method** `new()`: Creates a new instance of this R6 class.

 USAGE:

```r
Objective$new(
   id = "f",
   properties = character(),
   domain,
   codomain = ps(y = p_dbl(tags = "minimize")),
   constants = ps(),
   check_values = TRUE
)
```

**Arguments:**

- `id` (character(1)).
- `properties` (character()).
- `domain` (paradox::ParamSet)
   Specifies domain of function. The paradox::ParamSet should describe all possible input parameters of the objective function. This includes their id, their types and the possible range.
- `codomain` (paradox::ParamSet)
   Specifies codomain of function. Most importantly the tags of each output "Parameter" define whether it should be minimized or maximized. The default is to minimize each component.
- `constants` (paradox::ParamSet)
   Changeable constants or parameters that are not subject to tuning can be stored and accessed here.
- `check_values` (logical(1))
   Should points before the evaluation and the results be checked for validity?

**Method** `format()`: Helper for print outputs.
Objective

Usage:
Objective$format()

Returns: character().

Method print(): Print method.

Usage:
Objective$print()

Returns: character().

Method eval(): Evaluates a single input value on the objective function. If check_values = TRUE, the validity of the point as well as the validity of the result is checked.

Usage:
Objective$eval(xs)

Arguments:
xs (list())
   A list that contains a single x value, e.g. list(x1 = 1, x2 = 2).

Returns: list() that contains the result of the evaluation, e.g. list(y = 1). The list can also contain additional named entries that will be stored in the archive if called through the OptimInstance. These extra entries are referred to as extras.

Method eval_many(): Evaluates multiple input values on the objective function. If check_values = TRUE, the validity of the points as well as the validity of the results are checked. bbook does not take care of parallelization. If the function should make use of parallel computing, it has to be implemented by deriving from this class and overwriting this function.

Usage:
Objective$eval_many(xss)

Arguments:
xss (list())
   A list of lists that contains multiple x values, e.g. list(list(x1 = 1, x2 = 2), list(x1 = 3, x2 = 4)).

Returns: data.table::data.table() that contains one y-column for single-criteria functions and multiple y-columns for multi-criteria functions, e.g. `data.table(y = 1:2)` or `data.table(y1 = 1:2, y2 = 3:4)`. It may also contain additional columns that will be stored in the archive if called through the OptimInstance. These extra columns are referred to as extras.

Method eval_dt(): Evaluates multiple input values on the objective function

Usage:
Objective$eval_dt(xdt)

Arguments:
xdt (data.table::data.table())
   Set of untransformed points / points from the search space. One point per row, e.g. `data.table(x1 = c(1, 3), x2 = c(2, 4))`. Column names have to match ids of the search_space. However, xdt can contain additional columns.
**ObjectiveRFun**

Returns: data.table::data.table() that contains one y-column for single-criteria functions and multiple y-columns for multi-criteria functions, e.g. data.table(y = 1:2) or data.table(y1 = 1:2, y2 = 3:4).

**Method clone():** The objects of this class are cloneable with this method.

**Usage:**
Objective$clone(deep = FALSE)

**Arguments:**
deep Whether to make a deep clone.

---

**Description**

Objective interface where the user can pass a custom R function that expects a list as input. If the return of the function is unnamed, it is named with the ids of the codomain.

**Super class**

bbotk::Objective -> ObjectiveRFun

**Active bindings**

fun (function)
Objective function.

**Methods**

**Public methods:**

- ObjectiveRFun$new()
- ObjectiveRFun$eval()
- ObjectiveRFun$clone()

**Method new():** Creates a new instance of this R6 class.

**Usage:**
ObjectiveRFun$new(
  fun,
  domain,
  codomain = NULL,
  id = "function",
  properties = character(),
  constants = ps(),
  check_values = TRUE
)
**Arguments:**

fun (function)

- R function that encodes objective and expects a list with the input for a single point (e.g. `list(x1 = 1, x2 = 2)`) and returns the result either as a numeric vector or a list (e.g. `list(y = 3)`).

domain (paradox::ParamSet)

- Specifies domain of function. The paradox::ParamSet should describe all possible input parameters of the objective function. This includes their id, their types and the possible range.

codomain (paradox::ParamSet)

- Specifies codomain of function. Most importantly the tags of each output “Parameter” define whether it should be minimized or maximized. The default is to minimize each component.

id (character(1)).

properties (character()).

constants (paradox::ParamSet)

- Changeable constants or parameters that are not subject to tuning can be stored and accessed here.

check_values (logical(1))

- Should points before the evaluation and the results be checked for validity?

**Method** eval(): Evaluates input value(s) on the objective function. Calls the R function supplied by the user.

*Usage:*

`ObjectiveRFun$eval(xs)`

*Arguments:*

xs Input values.

**Method** clone(): The objects of this class are cloneable with this method.

*Usage:*

`ObjectiveRFun$clone(deep = FALSE)`

*Arguments:*

deep Whether to make a deep clone.

**Examples**

```r
# define objective function
fun = function(xs) {
  -(xs[[1]] - 2)^2 - (xs[[2]] + 3)^2 + 10
}

# set domain
domain = ps(
  x1 = p_dbl(-10, 10),
  x2 = p_dbl(-5, 5)
)
```
# set codomain
codomain = ps(y = p_dbl(tags = "maximize"))

# create Objective object
obfun = ObjectiveRFun$new(
  fun = fun,
  domain = domain,
  codomain = codomain,
  properties = "deterministic"
)

ObjectiveRFunDt  Objective interface for basic R functions.

Description

Objective interface where user can pass an R function that works on an data.table().

Super class

bbotk::Objective -> ObjectiveRFunDt

Active bindings

fun (function)
  Objective function.

Methods

Public methods:
- ObjectiveRFunDt$new()
- ObjectiveRFunDt$eval_many()
- ObjectiveRFunDt$eval_dt()
- ObjectiveRFunDt$clone()

Method new(): Creates a new instance of this R6 class.

Usage:

ObjectiveRFunDt$new(
  fun,
  domain,
  codomain = NULL,
  id = "function",
  properties = character(),
  constants = ps(),
  check_values = TRUE
)

Arguments:
fun (function)
R function that encodes objective and expects an \texttt{data.table()} as input whereas each point is represented by one row.

domain (\texttt{paradox::ParamSet})
Specifies domain of function. The \texttt{paradox::ParamSet} should describe all possible input parameters of the objective function. This includes their id, their types and the possible range.

codomain (\texttt{paradox::ParamSet})
Specifies codomain of function. Most importantly the tags of each output "Parameter" define whether it should be minimized or maximized. The default is to minimize each component.

\texttt{id (character(1)).}
\texttt{properties (character()).}
\texttt{constants (paradox::ParamSet)}
Changeable constants or parameters that are not subject to tuning can be stored and accessed here.

\texttt{check_values (logical(1))}
Should points before the evaluation and the results be checked for validity?

\textbf{Method} \texttt{eval_many()}:
Evaluates multiple input values received as a list, converted to a \texttt{data.table()} on the objective function. Missing columns in \texttt{xss} are filled with \texttt{NAs} in \texttt{xdt}.

\textit{Usage:}
\texttt{ObjectiveRFunDt$eval_many(xss)}

\textit{Arguments:}
\texttt{xss (list())}
A list of lists that contains multiple x values, e.g. \texttt{list(list(x1 = 1, x2 = 2), list(x1 = 3, x2 = 4))}.

\textit{Returns:} \texttt{data.table::data.table()} that contains one y-column for single-criteria functions and multiple y-columns for multi-criteria functions, e.g. \texttt{data.table(y = 1:2)} or \texttt{data.table(y1 = 1:2, y2 = 3:4)}.

\textbf{Method} \texttt{eval_dt()}:
Evaluates multiple input values on the objective function supplied by the user.

\textit{Usage:}
\texttt{ObjectiveRFunDt$eval_dt(xdt)}

\textit{Arguments:}
\texttt{xdt (data.table::data.table())}
Set of untransformed points / points from the \textit{search space}. One point per row, e.g. \texttt{data.table(x1 = c(1, 3), x2 = c(2, 4))}. Column names have to match ids of the \textit{search space}. However, \texttt{xdt} can contain additional columns.

\textit{Returns:} \texttt{data.table::data.table()} that contains one y-column for single-criteria functions and multiple y-columns for multi-criteria functions, e.g. \texttt{data.table(y = 1:2)} or \texttt{data.table(y1 = 1:2, y2 = 3:4)}.

\textbf{Method} \texttt{clone()}:
The objects of this class are cloneable with this method.
opt

Syntactic Sugar Optimizer Construction

Description

This function complements mlr_optimizers with functions in the spirit of mlr_sugar from mlr3.

Usage

opt(.key, ...)
opts(.keys, ...)

Arguments

.key
(character(1))
Key passed to the respective dictionary to retrieve the object.

... (named list())
Named arguments passed to the constructor, to be set as parameters in the paradox::ParamSet, or to be set as public field. See mlr3misc::dictionary_sugar_get() for more details.

.keys (character())
Keys passed to the respective dictionary to retrieve multiple objects.

Value

- Optimizer for opt().
- list of Optimizer for opts().

Examples

opt("random_search", batch_size = 10)
Description

Abstract base class.

Technical details

The Optimizer writes the final result to the .result field by using the $assign_result() method. .result stores a data.table::data.table consisting of x values in the search space, (transformed) x values in the domain space and y values in the codomain space of the Objective. The user can access the results with active bindings (see below).

Public fields

objective (Objective).
search_space (paradox::ParamSet).
terminator (Terminator).
archive (Archive).
progressor (progressor())
    Stores progressor function.
ojective_multiplicator (integer()).

Active bindings

result (data.table::data.table)
    Get result
result_x_search_space (data.table::data.table)
    x part of the result in the search space.
result_x_domain (list())
    (transformed) x part of the result in the domain space of the objective.
result_y (numeric())
    Optimal outcome.
is_terminated (logical(1)).

Methods

Public methods:

• OptimInstance$new()
• OptimInstance$format()
• OptimInstance$print()
• OptimInstance$eval_batch()
• OptimInstance$assign_result()
• OptimInstance$objective_function()
• OptimInstance$clear()
• OptimInstance$clone()

**Method new():** Creates a new instance of this R6 class.

*Usage:*
OptimInstance$new(
  objective,
  search_space = NULL,
  terminator,
  keep_evals = "all",
  check_values = TRUE
)

*Arguments:*
objective (Objective).
search_space (paradox::ParamSet)
  Specifies the search space for the Optimizer. The paradox::ParamSet describes either a subset of the domain of the Objective or it describes a set of parameters together with a trafo function that transforms values from the search space to values of the domain.
  Depending on the context, this value defaults to the domain of the objective.
terminator (Terminator).
keep_evals (character(1))
  Keep all or only best evaluations in archive?
check_values (logical(1))
  Should x-values that are added to the archive be checked for validity? Search space that is logged into archive.

**Method format():** Helper for print outputs.

*Usage:*
OptimInstance$format()

**Method print():** Printer.

*Usage:*
OptimInstance$print(...)

*Arguments:*
... (ignored).

**Method eval_batch():** Evaluates all input values in xdt by calling the Objective. Applies possible transformations to the input values and writes the results to the Archive.
Before each batch-evaluation, the Terminator is checked, and if it is positive, an exception of class terminated_error is raised. This function should be internally called by the Optimizer.

*Usage:*
OptimInstance$eval_batch(xdt)

*Arguments:*

Method assign_result(): The Optimizer object writes the best found point and estimated performance value here. For internal use.

Usage:
OptimInstance$assign_result(xdt, y)

Arguments:
- xdt (data.table::data.table())
  x values as data.table() with one row. Contains the value in the search space of the OptimInstance object. Can contain additional columns for extra information.
- y (numeric(1))
  Optimal outcome.

Method objective_function(): Evaluates (untransformed) points of only numeric values. Returns a numeric scalar for single-crit or a numeric vector for multi-crit. The return value(s) are negated if the measure is maximized. Internally, $eval_batch() is called with a single row. This function serves as a objective function for optimizers of numeric spaces - which should always be minimized.

Usage:
OptimInstance$objective_function(x)

Arguments:
- x (numeric())
  Untransformed points.

Returns: Objective value as numeric(1), negated for maximization problems.

Method clear(): Reset terminator and clear all evaluation results from archive and results.

Usage:
OptimInstance$clear()

Method clone(): The objects of this class are cloneable with this method.

Usage:
OptimInstance$clone(deep = FALSE)

Arguments:
- deep Whether to make a deep clone.
OptimInstanceMultiCrit

Optimization Instance with budget and archive

Description

Wraps a multi-criteria Objective function with extra services for convenient evaluation. Inherits from OptimInstance.

- Automatic storing of results in an Archive after evaluation.
- Automatic checking for termination. Evaluations of design points are performed in batches. Before a batch is evaluated, the Terminator is queried for the remaining budget. If the available budget is exhausted, an exception is raised, and no further evaluations can be performed from this point on.

Super class

bbotk::OptimInstance -> OptimInstanceMultiCrit

Active bindings

result_x_domain (list())
  (transformed) x part of the result in the domain space of the objective.

result_y (numeric(1))
  Optimal outcome.

Methods

Public methods:

- OptimInstanceMultiCrit$new()
- OptimInstanceMultiCrit$assign_result()
- OptimInstanceMultiCrit$clone()

Method new(): Creates a new instance of this R6 class.

Usage:

OptimInstanceMultiCrit$new(
  objective,
  search_space = NULL,
  terminator,
  keep_evals = "all",
  check_values = TRUE
)

Arguments:

objective (Objective).
search_space (paradox::ParamSet)
   Specifies the search space for the Optimizer. The paradox::ParamSet describes either a subset of the domain of the Objective or it describes a set of parameters together with a trafo function that transforms values from the search space to values of the domain. Depending on the context, this value defaults to the domain of the objective.

terminator (Terminator)
   Multi-criteria terminator.
keep_evals (character(1))
   Keep all or only best evaluations in archive?
check_values (logical(1))
   Should x-values that are added to the archive be checked for validity? Search space that is logged into archive.

Method assign_result(): The Optimizer object writes the best found points and estimated performance values here (probably the Pareto set / front). For internal use.

Usage:
OptimInstanceMultiCrit$assign_result(xdt, ydt)

Arguments:
xdt (data.table::data.table())
   Set of untransformed points / points from the search space. One point per row, e.g. data.table(x1 = c(1, 3), x2 = c(2, 4)). Column names have to match ids of the search_space. However, xdt can contain additional columns.
ydt (numeric(1))
   Optimal outcomes, e.g. the Pareto front.

Method clone(): The objects of this class are cloneable with this method.

Usage:
OptimInstanceMultiCrit$clone(deep = FALSE)

Arguments:
deep Whether to make a deep clone.

OptimInstanceSingleCrit
   Optimization Instance with budget and archive

Description

Wraps a single-criteria Objective function with extra services for convenient evaluation. Inherits from OptimInstance.

- Automatic storing of results in an Archive after evaluation.
- Automatic checking for termination. Evaluations of design points are performed in batches. Before a batch is evaluated, the Terminator is queried for the remaining budget. If the available budget is exhausted, an exception is raised, and no further evaluations can be performed from this point on.
Super class

bbotk::OptimInstance -> OptimInstanceSingleCrit

Methods

Public methods:

• OptimInstanceSingleCrit$new()
• OptimInstanceSingleCrit$assign_result()
• OptimInstanceSingleCrit$clone()

Method new(): Creates a new instance of this R6 class.

Usage:
OptimInstanceSingleCrit$new(
  objective,
  search_space = NULL,
  terminator,
  keep_evals = "all",
  check_values = TRUE
)

Arguments:

objective (Objective).

search_space (paradox::ParamSet)
  Specifies the search space for the Optimizer. The paradox::ParamSet describes either a 
  subset of the domain of the Objective or it describes a set of parameters together with 
  a trafo function that transforms values from the search space to values of the domain. 
  Depending on the context, this value defaults to the domain of the objective.

terminator (Terminator).

keep_evals (character(1))
  Keep all or only best evaluations in archive?

check_values (logical(1))
  Should x-values that are added to the archive be checked for validity? Search space that is 
  logged into archive.

Method assign_result(): The Optimizer object writes the best found point and estimated 
performance value here. For internal use.

Usage:
OptimInstanceSingleCrit$assign_result(xdt, y)

Arguments:

xdt (data.table::data.table())
  Set of untransformed points / points from the search space. One point per row, e.g. data.table(x1 
  = c(1, 3), x2 = c(2, 4)). Column names have to match ids of the search_space. How-
  ever, xdt can contain additional columns.

y (numeric(1))
  Optimal outcome.

Method clone(): The objects of this class are cloneable with this method.
Usage:
OptimInstanceSingleCrit$clone(deep = FALSE)

Arguments:
depth Whether to make a deep clone.

---

Description

Abstract Optimizer class that implements the base functionality each Optimizer subclass must provide. A Optimizer object describes the optimization strategy. A Optimizer object must write its result to the $assign_result() method of the OptimInstance at the end in order to store the best point and its estimated performance vector.

Progress Bars

$optimize() supports progress bars via the package progressr combined with a Terminator. Simply wrap the function in progressr::with_progress() to enable them. We recommend to use package progress as backend; enable with progressr::handlers("progress").

Public fields

- id (character(1))
  Identifier of the object. Used in tables, plot and text output.

Active bindings

- param_set paradox::ParamSet
  Set of control parameters.
- label (character(1))
  Label for this object. Can be used in tables, plot and text output instead of the ID.
- man (character(1))
  String in the format [pkg]:[topic] pointing to a manual page for this object. The referenced help package can be opened via method $help().
- param_classes (character())
  Supported parameter classes that the optimizer can optimize. Subclasses of paradox::Param.
- properties (character())
  Set of properties of the optimizer. Must be a subset of bbotk_reflections$optimizer_properties.
- packages (character())
  Set of required packages. A warning is signaled by the constructor if at least one of the packages is not installed, but loaded (not attached) later on-demand via requireNamespace().
Methods

Public methods:

- `Optimizer$new()`
- `Optimizer$format()`
- `Optimizer$print()`
- `Optimizer$help()`
- `Optimizer$optimize()`
- `Optimizer$clone()`

**Method new()**: Creates a new instance of this **R6** class.

*Usage:*

```r
Optimizer$new(
  id = "optimizer",
  param_set,
  param_classes,
  properties,
  packages = character(),
  label = NA_character_,
  man = NA_character_
)
```

*Arguments:*

- `id` (character(1))
  Identifier for the new instance.
- `param_set` (**paradox::ParamSet**)
  Set of control parameters.
- `param_classes` (character())
  Supported parameter classes that the optimizer can optimize. Subclasses of **paradox::Param**.
- `properties` (character())
  Set of properties of the optimizer. Must be a subset of **bbotk_reflections$optimizer_properties**.
- `packages` (character())
  Set of required packages. A warning is signaled by the constructor if at least one of the packages is not installed, but loaded (not attached) later on-demand via `requireNamespace()`.
- `label` (character(1))
  Label for this object. Can be used in tables, plot and text output instead of the ID.
- `man` (character(1))
  String in the format [pkg]:[topic] pointing to a manual page for this object. The referenced help package can be opened via method $help().

**Method format()**: Helper for print outputs.

*Usage:*

```r
Optimizer$format()
```

**Method print()**: Print method.

*Usage:*

```r
Optimizer$print()
```
Returns: (character()).

Method help(): Opens the corresponding help page referenced by field $man.

Usage:
Optimizer$help()

Method optimize(): Performs the optimization and writes optimization result into OptimInstance. The optimization result is returned but the complete optimization path is stored in Archive of OptimInstance.

Usage:
Optimizer$optimize(inst)

Arguments:
inst (OptimInstance).

Returns: data.table::data.table.

Method clone(): The objects of this class are cloneable with this method.

Usage:
Optimizer$clone(deep = FALSE)

Arguments:
deep Whether to make a deep clone.

Description

Wraps progressr::progressor() function and stores current progress.

Public fields

progressor (progressr::progressor()).
max_steps (integer(1)).
current_steps (integer(1)).
unit (character(1)).

Methods

Public methods:

• Progressor$new()
• Progressor$update()
• Progressor$clone()

Method new(): Creates a new instance of this R6 class.
Terminator

Usage:
Progressor$new(progressor, unit)

Arguments:
progressor (progressr::progressor())
    Progressor function.
unit (character(1))
    Unit of progress.

Method update(): Updates progressr::progressor() with current steps.

Usage:
Progressor$update(terminator, archive)

Arguments:
terminator (Terminator).
archive (Archive).

Method clone(): The objects of this class are cloneable with this method.

Usage:
Progressor$clone(deep = FALSE)

Arguments:
deep Whether to make a deep clone.

---

Terminator

Abstract Terminator Class

Description

Abstract Terminator class that implements the base functionality each terminator must provide. A terminator is an object that determines when to stop the optimization.

Termination of optimization works as follows:

- Evaluations in a instance are performed in batches.
- Before each batch evaluation, the Terminator is checked, and if it is positive, we stop.
- The optimization algorithm itself might decide not to produce any more points, or even might decide to do a smaller batch in its last evaluation.

Therefore the following note seems in order: While it is definitely possible to execute a fine-grained control for termination, and for many optimization algorithms we can specify exactly when to stop, it might happen that too few or even too many evaluations are performed, especially if multiple points are evaluated in a single batch (c.f. batch size parameter of many optimization algorithms). So it is advised to check the size of the returned archive, in particular if you are benchmarking multiple optimization algorithms.
Technical details

Terminator subclasses can overwrite .status() to support progress bars via the package \texttt{progressr}. The method must return the maximum number of steps (\texttt{max_steps}) and the currently achieved number of steps (\texttt{current_steps}) as a named integer vector.

Public fields

id (character(1))
   Identifier of the object. Used in tables, plot and text output.

Active bindings

\texttt{param\_set \ paradox::ParamSet}
   Set of control parameters.

\texttt{label (character(1))}
   Label for this object. Can be used in tables, plot and text output instead of the ID.

\texttt{man (character(1))}
   String in the format [\texttt{pkg}::\texttt{topic}] pointing to a manual page for this object. The referenced help package can be opened via method \texttt{$\text{help}()}.\n
\texttt{properties (character())}
   Set of properties of the terminator. Must be a subset of \texttt{bbotk\_reflections$terminator\_properties}.

\texttt{unit (character())}
   Unit of steps.

Methods

Public methods:

\begin{itemize}
\item \texttt{Terminator$new()}
\item \texttt{Terminator$format()}
\item \texttt{Terminator$print()}
\item \texttt{Terminator$status()}
\item \texttt{Terminator$remaining\_time()}
\item \texttt{Terminator$clone()}
\end{itemize}

Method \texttt{new()}: Creates a new instance of this \texttt{R6} class.

Usage:

\begin{verbatim}
Terminator$new(
   id, 
   param_set = ps(), 
   properties = character(), 
   unit = "percent", 
   label = NA_character_, 
   man = NA_character_ 
)
\end{verbatim}

Arguments:
id (character(1))
   Identifier for the new instance.

param_set (paradox::ParamSet)
   Set of control parameters.

properties (character())
   Set of properties of the terminator. Must be a subset of `bbotk_reflections$terminator_properties`.

unit (character())
   Unit of steps.

label (character(1))
   Label for this object. Can be used in tables, plot and text output instead of the ID.

man (character(1))
   String in the format `[pkg]::[topic]` pointing to a manual page for this object. The referenced help package can be opened via method `$help()`.

**Method** format(): Helper for print outputs.

*Usage*:
Terminator$format(with_params = FALSE)

*Arguments*:
with_params (logical(1))
   Add parameter values to format string.

**Method** print(): Printer.

*Usage*:
Terminator$print(...)

*Arguments*:
... (ignored).

**Method** status(): Returns how many progression steps are made (current_steps) and the amount steps needed for termination (max_steps).

*Usage*:
Terminator$status(archive)

*Arguments*:
archive (Archive).

*Returns*: named integer(2).

**Method** remaining_time(): Returns remaining runtime in seconds. If the terminator is not time-based, the remaining runtime is Inf.

*Usage*:
Terminator$remaining_time(archive)

*Arguments*:
archive (Archive).

*Returns*: integer(1).

**Method** clone(): The objects of this class are cloneable with this method.
### trm

**Usage:**
Terminator$clone(deep = FALSE)

**Arguments:**
deep Whether to make a deep clone.

**See Also**

---

**trm**  
*Syntactic Sugar Terminator Construction*

---

**Description**

This function complements `mlr_terminators` with functions in the spirit of `mlr_sugar` from `mlr3`.

**Usage**

```r
trm(.key, ...)
trms(.keys, ...)
```

**Arguments**

- **.key**  
  (character(1))
  Key passed to the respective `dictionary` to retrieve the object.

- **...**  
  (named list())
  Named arguments passed to the constructor, to be set as parameters in the `paradox::ParamSet`, or to be set as public field. See `mlr3misc::dictionary_sugar_get()` for more details.

- **.keys**  
  (character())
  Keys passed to the respective `dictionary` to retrieve multiple objects.

**Value**

- Terminator for `trm()`.
- list of Terminator for `trms()`.

**Examples**

```r
trm("evals", n_evals = 10)
```
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